An ab initio Study of Atomic Hydrogen Sorption on the Zigzag Edge of Pristine Bilayer Graphene

Raymund Bolalin1,2,*, Michelle Natividad1, Gerardo Janairo3, Hideaki Kasai4, and Nelson Arboleda Jr.1
1 Physics Department, De La Salle University, 2401 Taft Avenue, Manila
2 Applied Physics Department, EARIST, Nagtahan, Manila
3 Chemistry Department, De La Salle University, 2401 Taft Avenue, Manila
4 Division of Precision Science & Technology and Applied Physics, Osaka University, Japan
*Corresponding Author: raymund.bolalin@dlsu.ph

Abstract: We studied the sorption mechanism of atomic hydrogen on the zigzag edge of pristine bilayer graphene (BLG) as groundwork effort in the realization of the material’s utilization as the substrate in a hydrogen storage system. Using density functional theory, we performed total energy calculations, using pseudopotentials obtained from projector augmented wave (PAW) method. The Kohn-Sham equations were solved using plane waves with kinetic energies of 400 eV. The surface Brillouin zone integration was performed using the special-point sampling technique of Monkhorst and Pack (with \(4\times4\times1\) sampling meshes). For the exchange correlation energy, we adopted the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional. Each layer in the slab model we used in the calculations consisted of 28 sp\(^2\)-bonded carbon atoms with in-plane carbon-carbon distance of 1.42 Å and out-of-plane equilibrium stacking distance of 3.5 Å. Results revealed at least two non-activated reaction paths (paths of least potential) on pristine bilayer graphene which confirmed the possibility of absorbing H in between the carbon layers. Also, the strong H trap near the surface C atoms conveyed the strong tendency of C atoms to form sp\(^2\)p hybridization in the initial stage of H adsorption. The results suggest the possible utility of the zigzag edge as a reaction channel to carry out the sorption process.

Key Words: density functional theory; hydrogen; graphene; hydrogen storage; hydrogen fuel